

**Mathematical Modelling and
Simulation of Chemical Engineering Process
Professor Doctor Sourav Mondal
Department of Chemical Engineering
Indian Institute of Technology, Kharagpur
Lecture 8**

Partial differential equations – separation of variables

(Refer Slide Time: 00:46)

Case (ii)

$$u_t = u_{xx}$$

@ $u(t=0) = u_0$

@ $x=0, u_x=0$ & $x=1, u=0$

Consider $u = X(x)T(t)$

$$\Rightarrow X T_t = T X_{xx}$$

$$\Rightarrow \frac{1}{T} T_t = \frac{1}{X} X_{xx} = -\lambda^2$$

For x part, $X_{xx} + \lambda^2 X = 0$

$$\Rightarrow X = C_1 \sin(\lambda x) + C_2 \cos(\lambda x)$$

Hello everyone. So, now, we are going to proceed from where we left in the last class, that is regarding separation of variable technique for solution of linear PDEs, particularly parabolic PDEs. So, in this case as you know, that the case 2, where we have one of the conditions or one of the boundary conditions to be of Dirichlet type.

So, if you recall from the last class that one of the space boundary condition is the Neumann type and the other one is Dirichlet type. So, this is the difference we are having, that this boundary condition at x is equal to 0 we have set the derivative of that u to be equal to 0. And please note that in the main equation, I have dropped this α term today so, that you know what just for simplicity. So, we consider we follow the same approach. So, we consider u is equal to function of 2 linearly independent (you know) functions or product of 2 linearly independent functions and we get you place this equation, I mean use this substitution in the main equation. So, you get something like this.

Next, we set up the auxiliary equations and (you know) that from the last class only we have discussed that these two will be equal only in the case when it is negative constant quantity. So, we set up the auxiliary equations for x part and for the time parts of our x part it is sorry, is equal to 0 and the solution to which let me write it straight away $C_1 \sin \lambda x$ plus $C_2 \cos \lambda x$. Now, comes the interesting part is that, to find out the value of these constants C_1 and C_2 , you need the help of the boundary conditions.

(Refer Slide Time: 02:59)

Since $u_x = 0$ at $x = 0$

$$X = C_1 \sin(\lambda x) + C_2 \cos(\lambda x)$$

$$0 = X_x \Big|_{x=0} = C_1 \cos(\lambda x) + C_2 \sin(\lambda x)$$

$$\rightarrow X = C_2 \cos(\lambda x)$$

@ $x = 1, u = 0 \Rightarrow X = 0$

$$C_2 \cos(\lambda x) = 0$$

$$\lambda = \left(n + \frac{1}{2}\right) \pi \quad \text{where } n = 0, \pm 1, \pm 2, \dots$$

So, at x is equal to 0, since, u_x is equal to 0 at x is equal to 0 what we get from here is that our x is equal to $C_1 \sin \lambda x$ plus $C_2 \cos \lambda x$. So, if you take the derivative, if you try to do xx you are going to get a \cos term and a \sin term? So, something like $C_1 \cos$ and $C_2 \sin$ of this quantity and if you said that the value at x is equal to 0 is equal to 0. So, this implies that it is only possible when C_1 is equal to 0. So, from here using this boundary condition you get when C_1 is equal to 0, so, it becomes $C_2 \cos \lambda x$ and you know that at x is equal to 1 this u is equal to 0 which implies capital X is equal to 0.

So, this means that $C_2 \cos \lambda x$ is equal to 0 now. Clearly C_2 cannot be equal to 0, otherwise the space dependency will no longer exist. So, in that case the possible solution is that all the Eigen values of this λ . So, λ is equal to n plus half π , because you know the

cosine function set equal to 0 at the you know this half of the pi or the multiples of half so, where n could be all possible integer quantities, and so on.

(Refer Slide Time: 04:53)

$T_t + \lambda_n^2 T = 0$
 $\hookrightarrow T = C_3 \exp(-\lambda_n t)$
 Linear superposition of all possible solutions,
 $u = \sum u_n = \sum_{n=0}^{\infty} C_n \exp(-\lambda_n^2 t) \cos(\lambda_n x)$
 where $\lambda_n = (n + \frac{1}{2})\pi$
 $\& n = 0, \pm 1, \pm 2, \dots$

For the time part it is the same thing so, for time we have already framed the auxiliary equations instead of writing lambda, we can write lambda n because the values of lambda are dependent on the Eigen values n. So, this gives you the solution t is equal to C3 exponential minus lambda nt. Now, we do a linear superposition of all the possible solutions and that gives us something like this, n is equal to 0 to infinity. So far everything is clear. So, now it is time to use the initial condition to evaluate out what would be the possible value of Cn.

(Refer Slide Time: 06:23)

Evaluating C_n using IC @ $t=0, u=u_0$

$$u_0 = \sum C_n \cos(\lambda_n x)$$

Orthogonality of cosine functions,

$$\int_0^1 u_0 \cos(\lambda_m x) = \int_0^1 \sum C_n \cos(\lambda_m x) \cos(\lambda_n x) dx$$

$m=n$ \Rightarrow $u_0 \frac{\sin(\lambda_n x)}{\lambda_n} \Big|_0^1 = C_n \int_0^1 \cos^2(\lambda_n x) dx$

$$\Rightarrow C_n = \frac{2 u_0 \sin(\lambda_n x)}{\lambda_n}$$

NPTEL

So, with the help of this initial condition which tells you that at t is equal to 0, u is equal to u_0 . So, it means u_0 something like this. So, use the orthogonality of cosine functions once again like in the last lecture, we discussed that all the trigonometric functions are orthogonal in nature. So, in this case the cosine functions. So, we multiply both sides with $\cos m \pi x$. So, we multiply both sides with \cos , sorry.

Let us not let us not write $m \pi x$ because it is m plus half πx so, instead better to write λ_n m , so, λ_n is like m plus half and λ_n is m plus half something like that, and we integrate over 0 to 1. Now clearly on the right-hand side all the terms should be equal to 0 except, for the case when m and n is equal.

So, using these criteria we evaluate the, I mean the left-hand side is straightforward integration. So, instead of n , I can write to be m , I can write to be n , is not it. So, m and n are equal only then the right hand side those term will only exist. So, the summation sign will go away and we will have both this m and n to be equal. So, of course, this right-hand side is equal to C_n by 2. So, overall this gives us C_n equal to $2 u_0 \sin$. So, this is the expression of our C_n .

(Refer Slide Time: 08:53)

Hence,

$$u = 2 u_0 \sum_{n=0}^{\infty} \frac{\sin(\lambda_n)}{\lambda_n} \exp(-\lambda_n^2 t) \cos(\lambda_n x)$$

where $\lambda_n = (n + \frac{1}{2})\pi \forall n = 0, \pm 1, \pm 2$

Now, we include this in the means, I mean the final solution, so, we get u is equal to u_0 ... So, I hope all of you can spot the difference in the initial constants as well as instead of a sin function now, we are having a cosine function from the change in the boundary conditions from Dirichlet to Neumann.

(Refer Slide Time: 09:57)

Case (iii) $u_t = u_{xx}$
 @ $t=0, u = u_0$
 @ $x=0, u=0$ & $x=1, u_x + \beta u = 0$

Consider $u = T(t)X(x)$
 $\Rightarrow \frac{1}{T} T_t = \frac{1}{X} X_{xx} = -\lambda^2$

for x -part $X_{xx} + \lambda^2 X = 0$
 $\Rightarrow X = C_1 \sin(\lambda x) + C_2 \cos(\lambda x)$
 Since BC, $u(x=0) = 0$

So, now it is time to move to the third case, when we have the mixed boundary type conditions. Again, we drop the alpha term just for the sake of simplicity. So, t is equal to 0 it is a constant, but at x is equal to 1, we have that mixed boundary type conditions. We can as I have said you can consider this to be a scenario of you know the convective type boundary condition, possible due to you know balance of conductive heat transfer to the convective loss from the surface.

So, once again we consider u is equal to $T(t)$ and $X(x)$. So, separation of variables tells us that the auxiliary equations would look again same and you know that these two quantities will only be equal only when it is a negative constant. So, for X part we have sorry, please do not get mixed up with capital X and small x . And the solution to this part is again X is equal to $C_1 \sin \lambda x$ plus $C_2 \cos \lambda x$.

Now, this would be equal to 0 because you can clearly understand from the boundary condition that u at x is equal to 0 is equal to 0, and this means that C_2 cannot exist. Otherwise, it will not satisfy the boundary condition. So, this tells us that C_2 sorry, this solution to the space part is only this much, with only the sin term.

(Refer Slide Time: 12:11)

$$\text{@ } x=1, \quad X_x + \beta X = 0 \quad \text{(Substitute } X = C_1 \sin(\lambda x)$$

$$\text{From this condition @ } x=1: \quad \lambda_1 + \beta \tan \lambda_1 = 0$$

transcendental eqn.

$$X_n = C_1 \sin(\lambda_n x)$$

$$T_n = C_2 \exp(-\lambda_n^2 t)$$

$$u_n = \sum X_n T_n$$

$$= \sum C_n \exp(-\lambda_n^2 t) \sin(\lambda_n x)$$

Now, we move to the you know this other boundary condition which tells us that at x is equal to 1 we have this $X_x + \beta x$. So, from this condition what we get, if you substitute, I mean the solution the x is equal to $C_1 \sin \lambda x$, then this gives you from this condition something like this, this is evaluated at x is equal to 1.

Now, this is an important transcendental equation because explicitly you cannot find out the values of your lambda. Like in the previous cases you easily get the values of lambda to be either $n\pi$ or $n + \text{half } \pi$, but in this case it is not an explicit solution of lambda. So is an implicit equation or sometimes it is called a transcendental equation and solution to which is possible by numerical techniques either you can use some bisection methods or some other techniques Newton Rapson technique to find out the different possible solutions of lambda.

You can also do a graphical construction and try to get this plot and see under what are the values for which it is intersecting the x axis. So, this is a transcendental type equation from where, transcendental equation from where you need to calculate or estimate the values of lambda. So, what we have we have X_n is equal to $C_1 \sin \lambda x$, where there is only values of the lambda should be obtained from that you transcendental equation and this is the time part we have. So, again we take the product of these two quantities. So u_n is equal to you know the summation of linear superposition of all the solutions. So, this gives us... so this should be summed over all the past possible values of lambda n .

(Refer Slide Time: 15:01)

$$\textcircled{a} \quad t=0, u=u_0 \Rightarrow u_0 = \sum C_n \sin(\lambda_n x)$$

$$\int_0^1 u_0 \sin(\lambda_n x) dx = \int_0^1 \sum C_n \sin(\lambda_n x) \sin(\lambda_m x) dx$$

$$u_0 \left[-\frac{\cos(\lambda_n x)}{\lambda_n} \right]_0^1 = C_n \int_0^1 \sin^2(\lambda_n x) dx$$

$$\sin 2x = \frac{2 \tan x}{1 + \tan^2 x}$$

$$I = \frac{1}{2} \left[1 - \frac{\sin(2\lambda_n)}{2\lambda_n} \right]$$

$$I = \frac{1}{2} \left[\frac{\beta + \beta^2 + \lambda_n^2}{\beta^2 + \lambda_n^2} \right]$$

$$\lambda_n + \beta \tan \lambda_n = 0$$

Now, once again it is time to use the initial conditions. So, at t is equal to 0 we have u is equal to u_0 . So, this means from the you know this combined solution we get use 0 is equal to summation of $C_n \sin \lambda x$. So, again we use the principle of orthogonality. So, what we get we multiply both sides with $\lambda_n x$ so, it is $u \sin \dots$. And the right hand side we also do the same thing. Do the integration, so the right hand side all the terms and all the different values of you know will be equal to 0 except for the case when n and m are equal.

So, this means the right hand side will have only those terms where m and n are equal and others will no longer exist. So, this is how the right hand side will going to look like and so, for cause this will evaluate the left hand side and this looks something like this. So, now this is slightly (you know) interesting and you can easily evaluate out what should be the integration constant here.

So, I think this you can find out, let us say this quantity, I mean C_n is a constant, so, I can write the integration inside this quantity and let us say this integration I . So, you can easily evaluate out what should be the integration of this $\sin^2 dx$. So, let me just write. So, you can do a simple quick expansion of $\sin 2x$. So, $\sin 2x$, let me use a different color, $\sin 2x$ can be expanded in you know a standard trigonometric form. So, $\sin 2x$ is equal to $2 \tan x$ by $1 + \tan^2 x$. I

am not doing the intermediate steps here, and if you do the substitution here you are going to get your I. This I will be transformed to something like this.

So, from where I am getting this? You already have this transcendental equation. So, the transcendental equation is already with you. So, that is $\lambda_n + \beta \tan \lambda_n = 0$, this is the transcendental equation, which you already have. So, using this equation, you just convert the $\sin 2\lambda_n$ and in terms of \tan quantities.

So, it had be easier to use this expression in the \tan form, that is the reason why I suggested that you use these trigonometric substitutions here and then apply the (you know) transcendental equation into this equation and finally, we will ending up with I something like this. I am not doing the intermediate steps; I hope that is something you will be able to do it.

(Refer Slide Time: 19:18)

$$u = 2u_0 \sum_{n=1}^{\infty} C_n \left[\frac{1 - \cos \lambda_n x}{\lambda_n} \right] \left[\frac{\beta^2 + \lambda_n^2}{\beta + \beta^2 + \lambda_n^2} \right] \exp(-\lambda_n^2 t) \sin(\lambda_n x)$$

$$\boxed{\lambda_n + \beta \tan(\lambda_n) = 0}$$

↓ $\lambda_1, \lambda_2, \lambda_3$ -----

So, the now the final solution comes to... So this is $\beta^2 \lambda_n^2 + \beta + \lambda_n^2$, guys please note that this entire part is actually I mean two into this quantity, is actually your C_n . So, this is you are actually C_n , without of course the extra summation sign and together with that you have the transcendental equation.

So, this will give you the solutions of different you know the values of lambda. So, these you can designate them as λ_1 , λ_2 , λ_3 , etc., the possible solutions this will also give you infinite solutions, and all the possible solutions should be fed here to this summation together and the linear superposition of all the terms will give you the final solution.

So, with this I would like to close the technique of separation of variables particularly for Cartesian systems. In the next lecture, we will see another example of a scenario where we have these cylindrical coordinate systems and possibly you would be landing up with Bessel functions solutions. So, I hope you liked this lecture today and you get a good idea about the technique of separation of variables and this is very useful for (you know) parabolic systems. We have only did the exercise we have done the exercise for the case of (you know) 1 dimensional in space, but this can also be (you know) extended for the case of (you know) 2 dimension systems. I hope you liked the lecture today. Thank you.